

GPR  
TabPFN  
GPT-SMILES  
GPT-Name  
GPT-InChI  
GPT-SELFIES

accuracy

0.8

0.6

0

50

100

150

200

$F_1$  macro

0.75

0.50

0

50

100

150

200

$F_1$  micro

0.8

0.6

0

50

100

150

200

$\kappa$

0.75

0.50

0.25

0

50

100

150

200

number of training points

